On connections between k-coloring and Euclidean k-means

Karthik C. S. (Rutgers University)



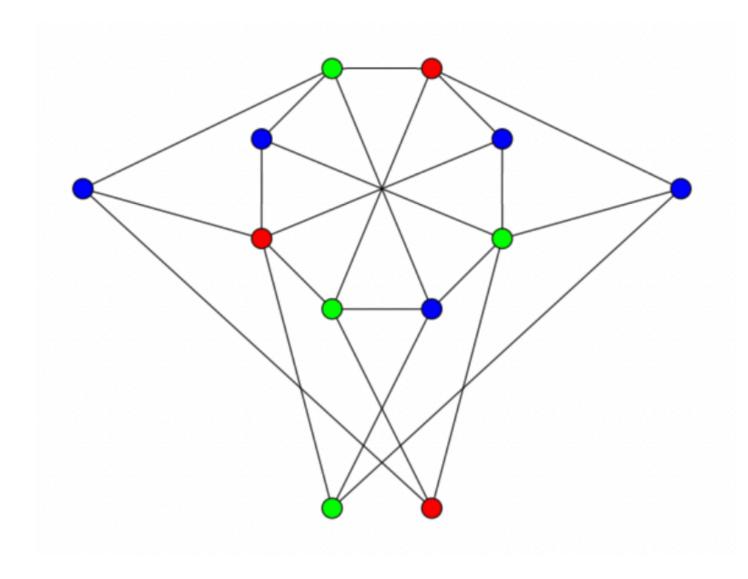
Enver Aman Undergrad at Rutgers Graduated May 2024

Joint Work with

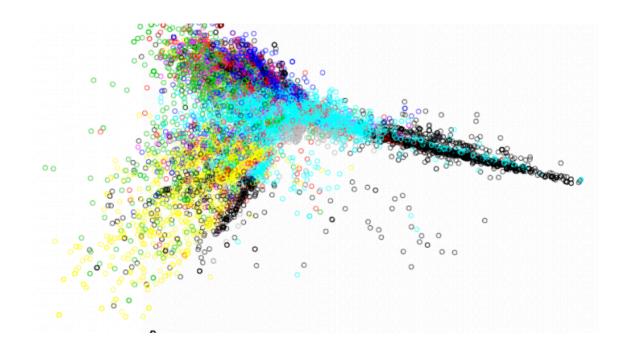




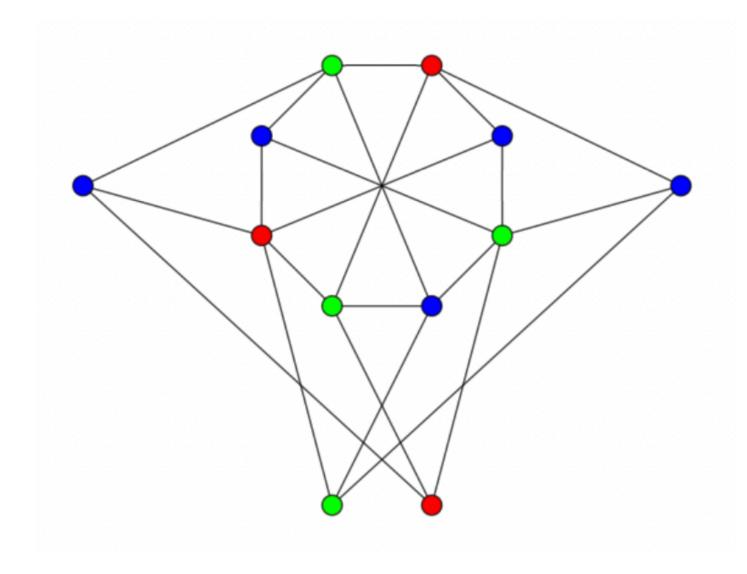
Sharath Punna Masters at Rutgers Graduated May 2023



k-means Clustering

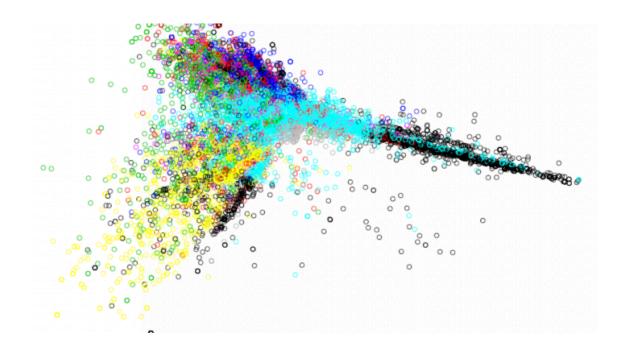


• Input: Graph G = (V, E) and integer k

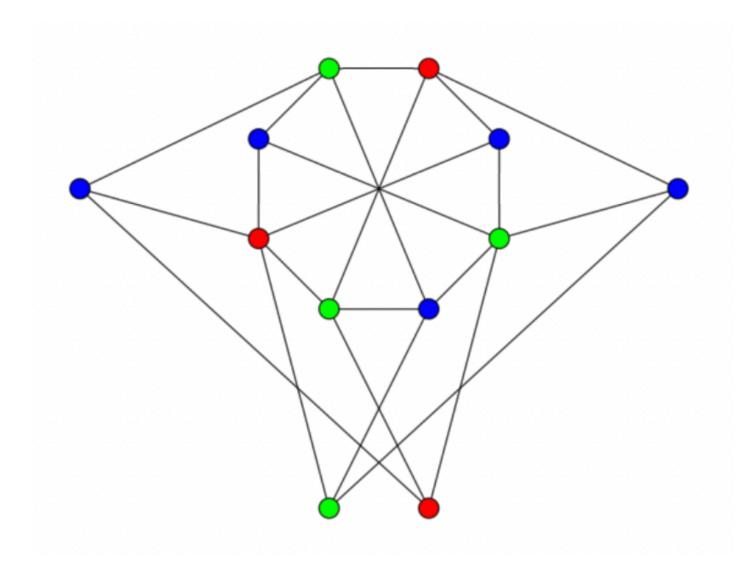


k-means Clustering

• Input: Points $P \subset \mathbb{R}^d$ and integer k



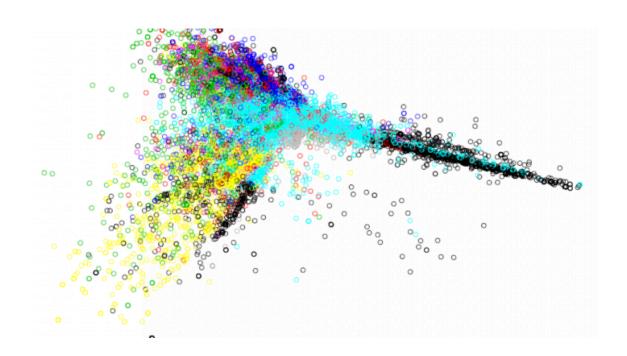
- Input: Graph G = (V, E) and integer k
- Output: $V := V_1 \dot{\cup} \cdots \dot{\cup} V_{k'}$ such that V_i is an independent set



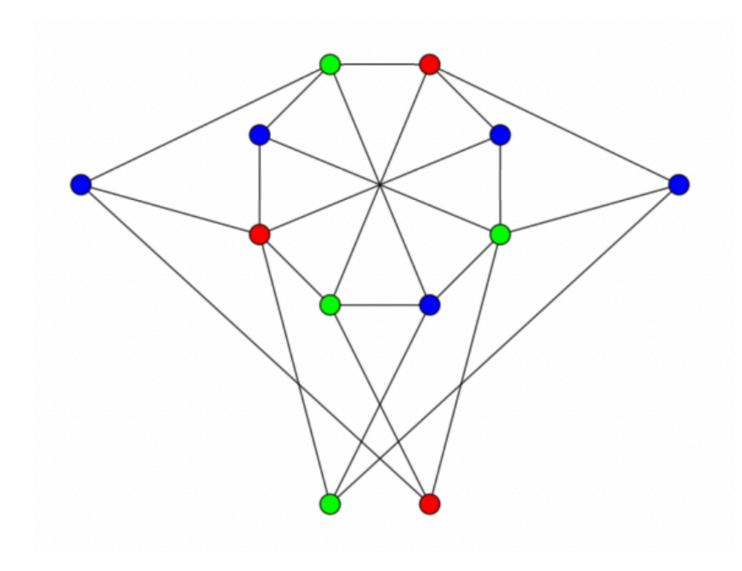
k-means Clustering

- Input: Points $P \subset \mathbb{R}^d$ and integer k
- Output: $P := P_1 \dot{\cup} \cdots \dot{\cup} P_{k'}$ such that

 $\sum_{i \in [k]} \sum_{p \in P_i} ||p - c_i||_2^2 \text{ is minimized,}$ where $c_i = \sum_{p \in P_i} \frac{p}{|P_i|}$

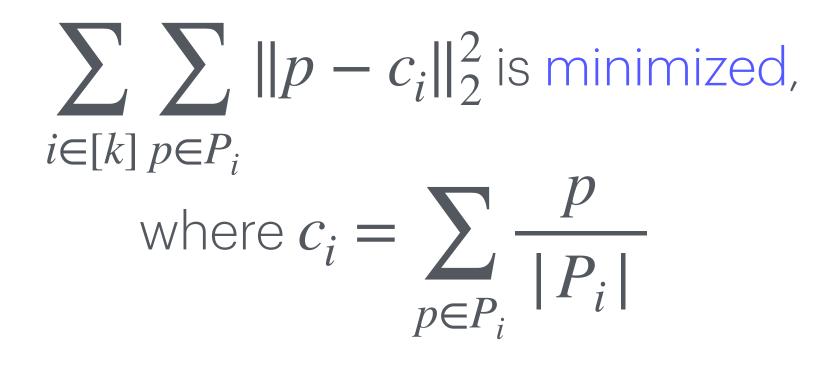


- Input: Graph G = (V, E) and integer k
- Output: $V := V_1 \dot{\cup} \cdots \dot{\cup} V_{k'}$ such that V_i is an independent set
- Classic NP-hard problem

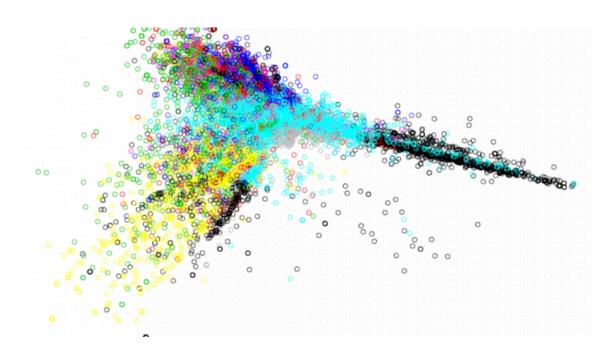


k-means Clustering

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Important NP-hard problem



Graph k-Coloring

• Input: Graph G = (V, E), G is d-regular

k-means Clustering

• Input: Points $P \subset \mathbb{R}^d$

Graph k-Coloring

• Input: Graph G = (V, E), G is d-regular

$$v \in V$$

$$p_{v}(e) = \begin{cases} +1\\ -1\\ 0 \end{cases}$$

k-means Clustering • Input: Points $P \subset \mathbb{R}^d$

Orient *E* arbitrarily

$\longrightarrow p_{v} \in \mathbb{R}^{|E|}$

if *e* is outgoing edge of *v* if *e* is incoming edge of *v* otherwise

Graph k-Coloring

• Input: Graph G = (V, E), G is d-regular

 $\{u,v\} \in E \implies 2d+2$ $\{u,v\} \in E \implies 2d+2$ $P_{u}\|_{2}^{2} = 4 + 2(d-1) = 2d+2$ NPv

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Graph k-Coloring

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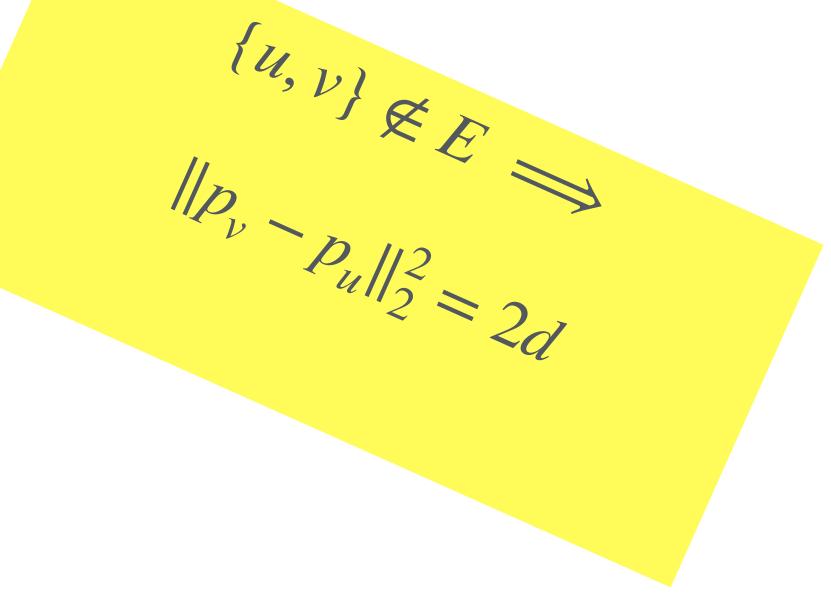
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Graph k-Coloring

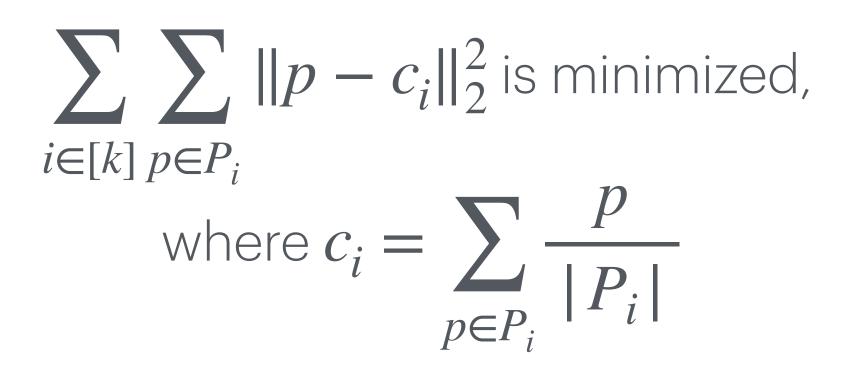
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k-means Clustering • Input: Points $P \subset \mathbb{R}^{|E|}$

 $\|p_u - p_v\|_2^2 = \begin{cases} 2d & \text{if } \{u, v\} \notin E \\ 2d + 2 & \text{if } \{u, v\} \in E \end{cases}$

Graph k-Coloring

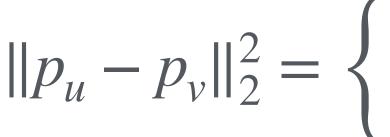
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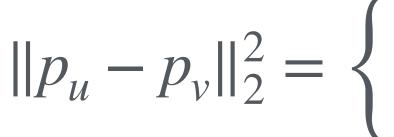
 $\sum_{i=1}^{n} \frac{1}{2|P_i|} \sum_{i=1}^{n} ||p-q||_2^2$ $i \in [k] \stackrel{\sim}{}^{i} \stackrel{i}{}^{i} p, q \in P_i$ is minimized,



Completeness

$\|p_u - p_v\|_2^2 = \begin{cases} 2d & \text{if } \{u, v\} \notin E \\ 2d + 2 & \text{if } \{u, v\} \in E \end{cases}$

Soundness



Completeness

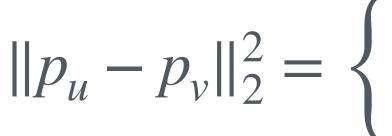
• $V := V_1 \dot{\cup} \cdots \dot{\cup} V_{k'}$ such that V_i is an independent set

 $i \in [k]$

$$\sum_{i \in [k]} \frac{1}{2|P_i|} \sum_{p,q \in P_i} \|p - q\|_2^2 = \sum_{i \in [k]} \frac{1}{2|P_i|} \sum_{p,q \in P_i} 2d$$
$$= \sum_{i \in [k]} d \cdot (|P_i| - 1) = d \cdot (|V| - k)$$

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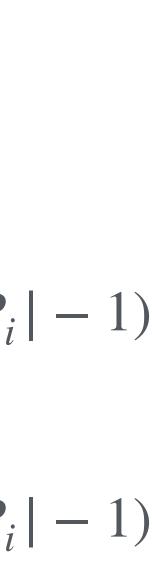
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Soundness • $P := P_1 \dot{\cup} \cdots \dot{\cup} P_k$ is some clustering . ∀*i* ∈ [*k*], $\sum_{i=1}^{n} ||p - q||_2^2 \ge 2d \cdot |P_i| \cdot (|P_i| - 1)$ $p,q \in P_i$ ∃*i* ∈ [*k*], $\sum \|p - q\|_2^2 > 2d \cdot |P_i| \cdot (|P_i| - 1)$

 $p,q \in P_i$

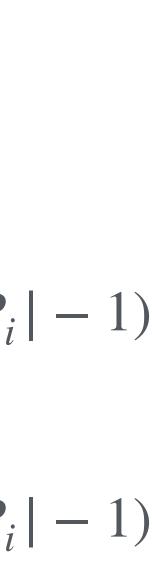


• $V := V_1 \dot{\cup} \cdots \dot{\cup} V_{k'}$ such that

•
$$\sum_{i \in [k]} \frac{1}{2|P_i|} \sum_{p,q \in P_i} ||p-q||_2^2 = \sum_{i \in [k]} \frac{1}{2|P_i|} \sum_{p,q \in P_i} 2d$$

 $= \sum d \cdot (|P_i| - 1) = d \cdot (|V| - k)$ $i \in [k]$

$\|p_{u} - p_{v}\|_{2}^{2} = \begin{cases} 2d & \text{if } \{u, v\} \notin E \\ 2d + 2 \\ d + 2$. ∀*i* ∈ [*k*], $\sum_{i=1}^{n} ||p - q||_2^2 \ge 2d \cdot |P_i| \cdot (|P_i| - 1)$ $p,q \in P_i$ $\exists i \in [k], \quad \sum \|p - q\|_2^2 > 2d \cdot |P_i| \cdot (|P_i| - 1)$ $p,q\in P_i$







- 2-coloring reduces to 2-means
- 2-coloring is in P so 2-means is in P



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• 2-means is NP-hard [Dasgupta-Freund'09]



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- Proof Strategy:

(i) Structured 3-NAE-SAT is NP-hard

(ii) NAE-SAT is reduced to distance matrix of points of 2-means instance

(iii) Distance matrix can be realized in Euclidean space (PSD check)

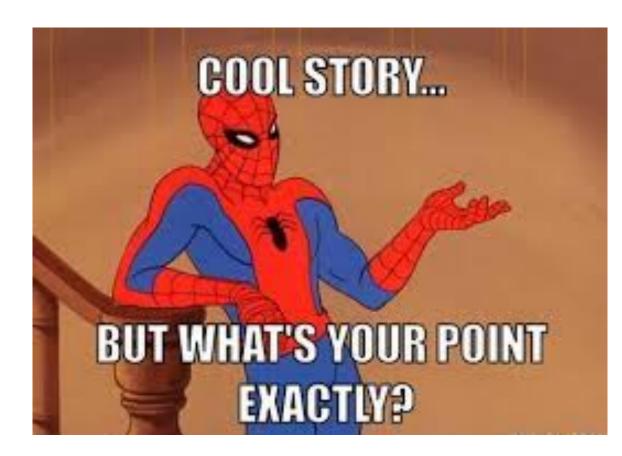


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Almost 2-coloring to 2-means

Almost 2-coloring to 2-means New Reduction

Balanced Max-Cut

- Input: Graph G = (V, E), G is d-regular
- Output: $V := V_1 \stackrel{.}{\cup} V_2$, to minimize:

$$|E \setminus E(V_1, V_2)| \cdot \left(1 + \frac{||V_1| - |V_2||}{|V|}\right)$$

2-means Clustering

- Input: Points $P \subset \mathbb{R}^d$
- Output: $P := P_1 \dot{\cup} P_2$, to minimize:

$$\frac{\sum_{p,q\in P_1} \|p-q\|_2^2}{2\|P_1\|} + \frac{\sum_{p,q\in P_2} \|p-q\|_2^2}{2\|P_2\|}$$

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Max-Cut on *n* vertices can be solved in $2^{\omega n/3}$ time

[Williams'05]

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2-means on n points can be solved in $2^{\omega n/3}$ time

This paper

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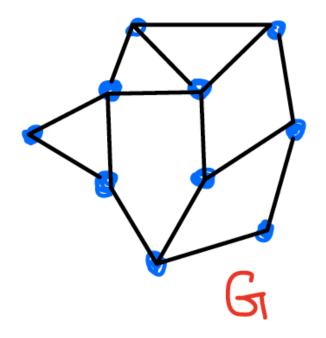
 $\frac{\text{State-of-the-art}}{2^{\omega n/3}} \le 1.73^n$

$\begin{array}{l} 2\text{-means on }n \text{ points}\\ \text{can be solved in}\\ 2^{\omega n/3} \text{ time} \end{array}$

This paper

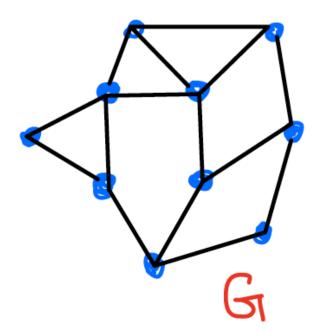
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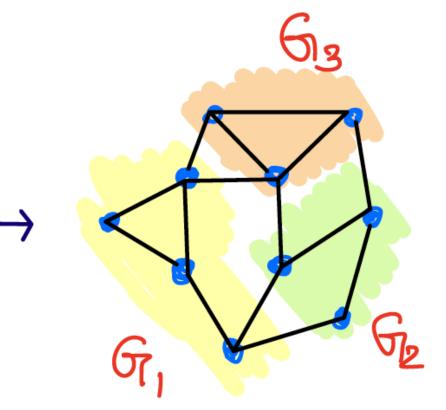
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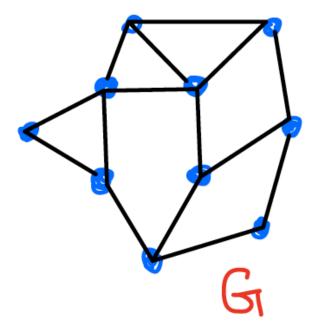


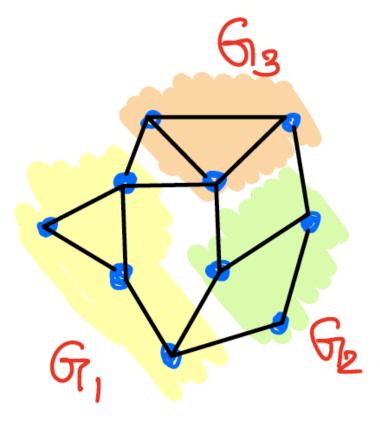


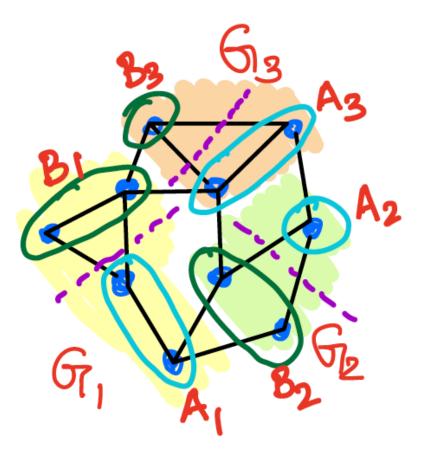
Max-Cut on *n* vertices can be solved in $2^{\omega n/3}$ time

[Williams'05]

• Enumerate all cuts (A_i, B_i) of G_i



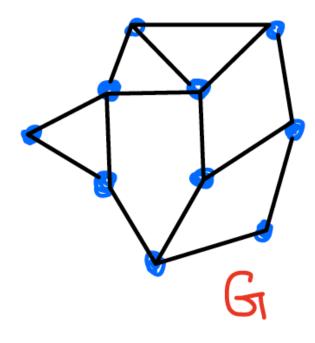


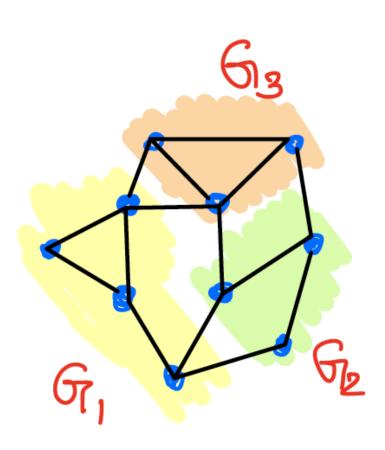


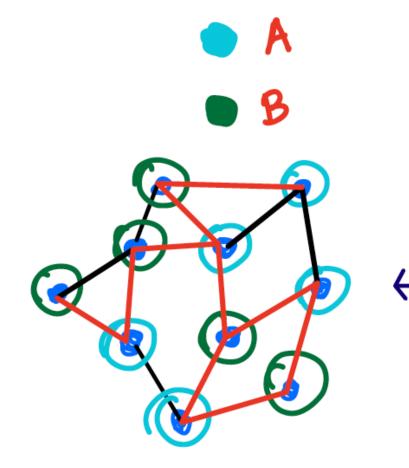
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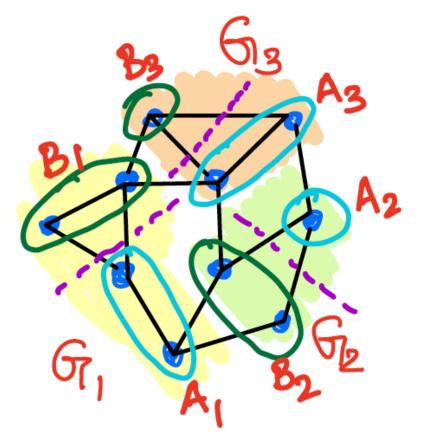
[Williams'05]

- Enumerate all cuts (A_i, B_i) of G_i
- Construct graph H on $3 \cdot 2^{n/3}$ nodes
- Edge Weight of H is sum of cut edges





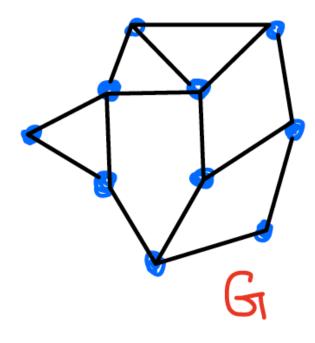


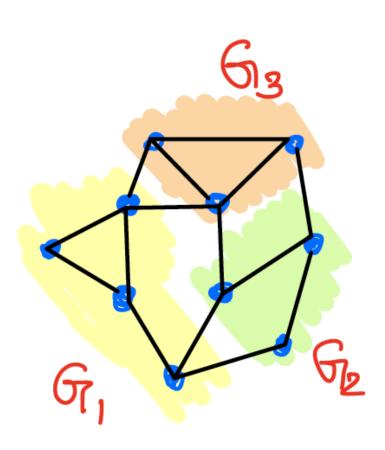


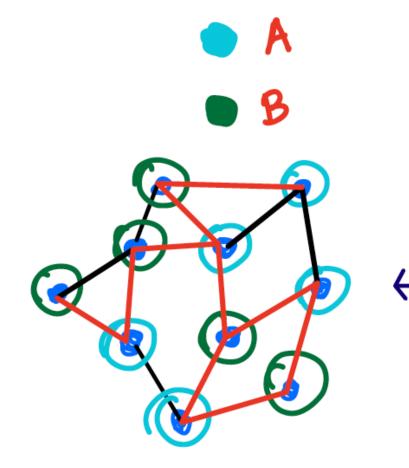
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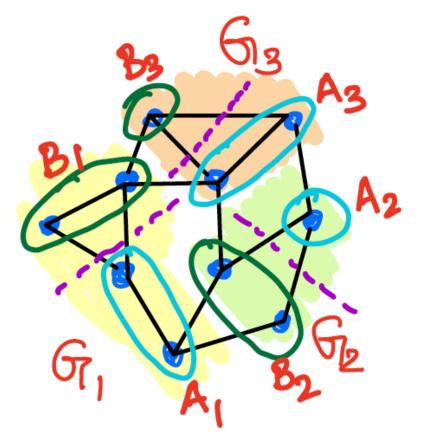
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- Enumerate all cuts (A_i, B_i) of G_i
- Construct graph H on $3 \cdot 2^{n/3}$ nodes
- Edge Weight of H is sum of cut edges
- Solve weighted triangle detection on $3\cdot 2^{n/3}$ node graph H



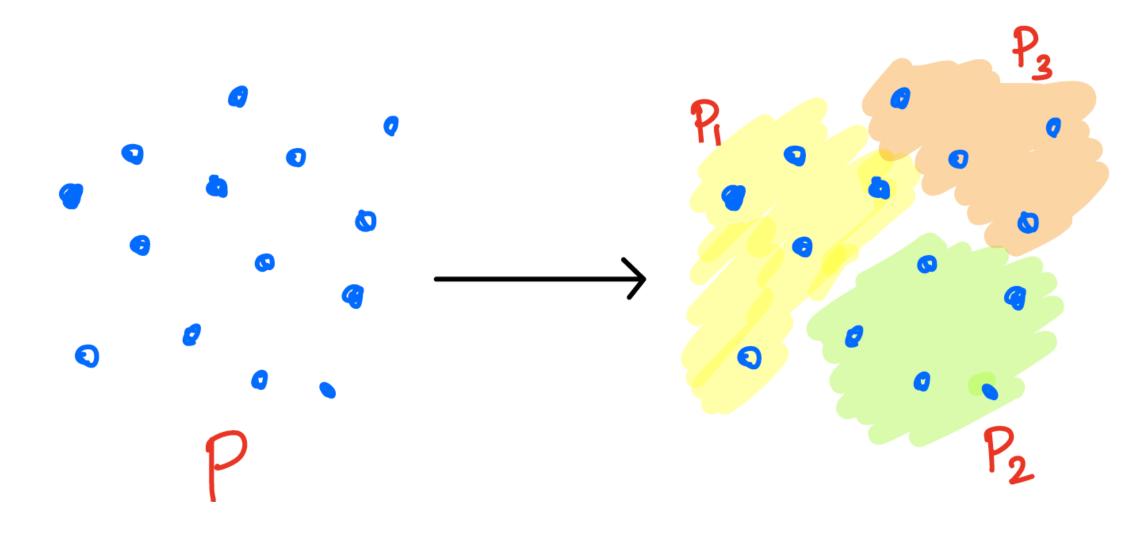






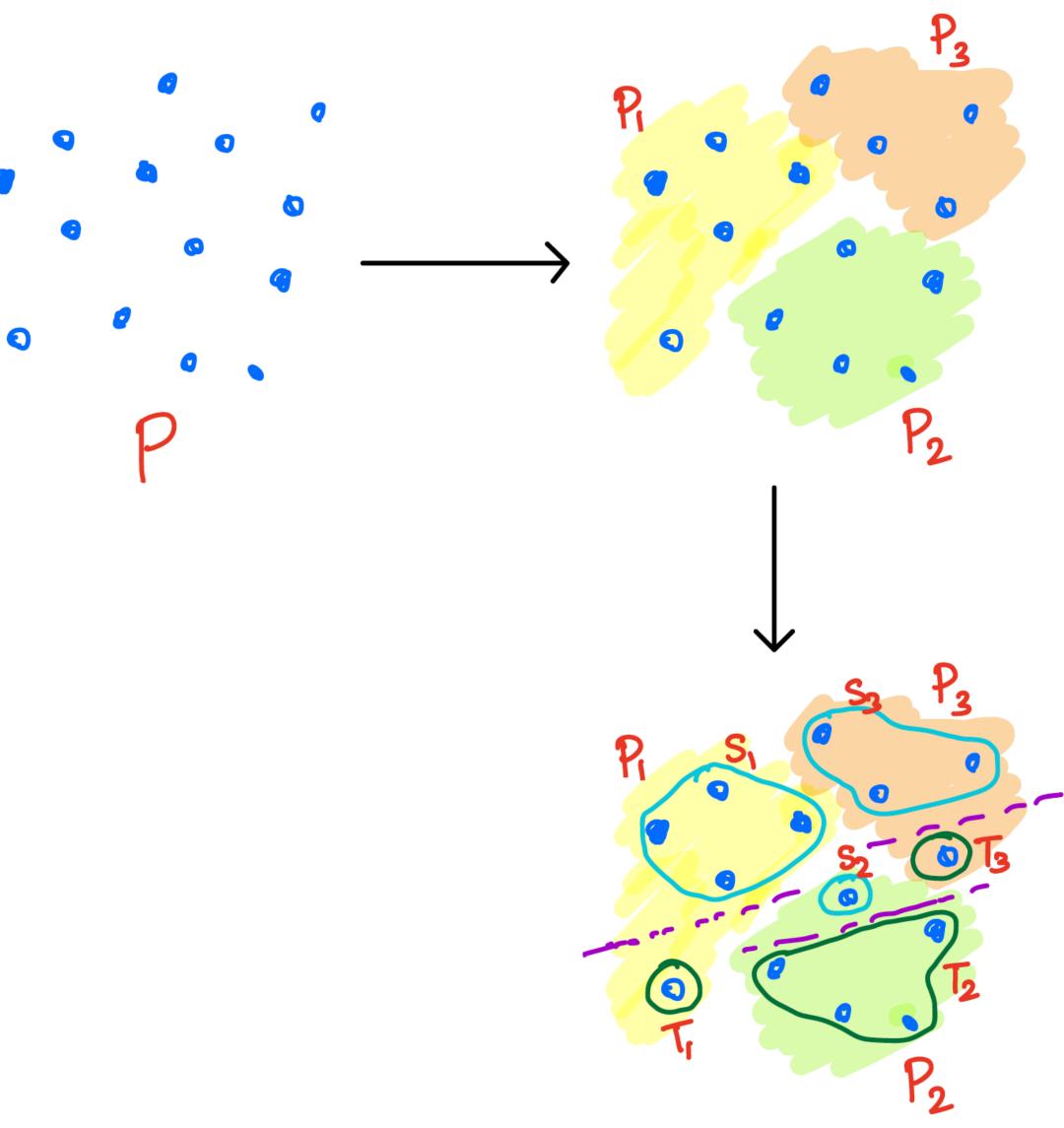
2-means on n points can be solved in $2^{\omega n/3}$ time

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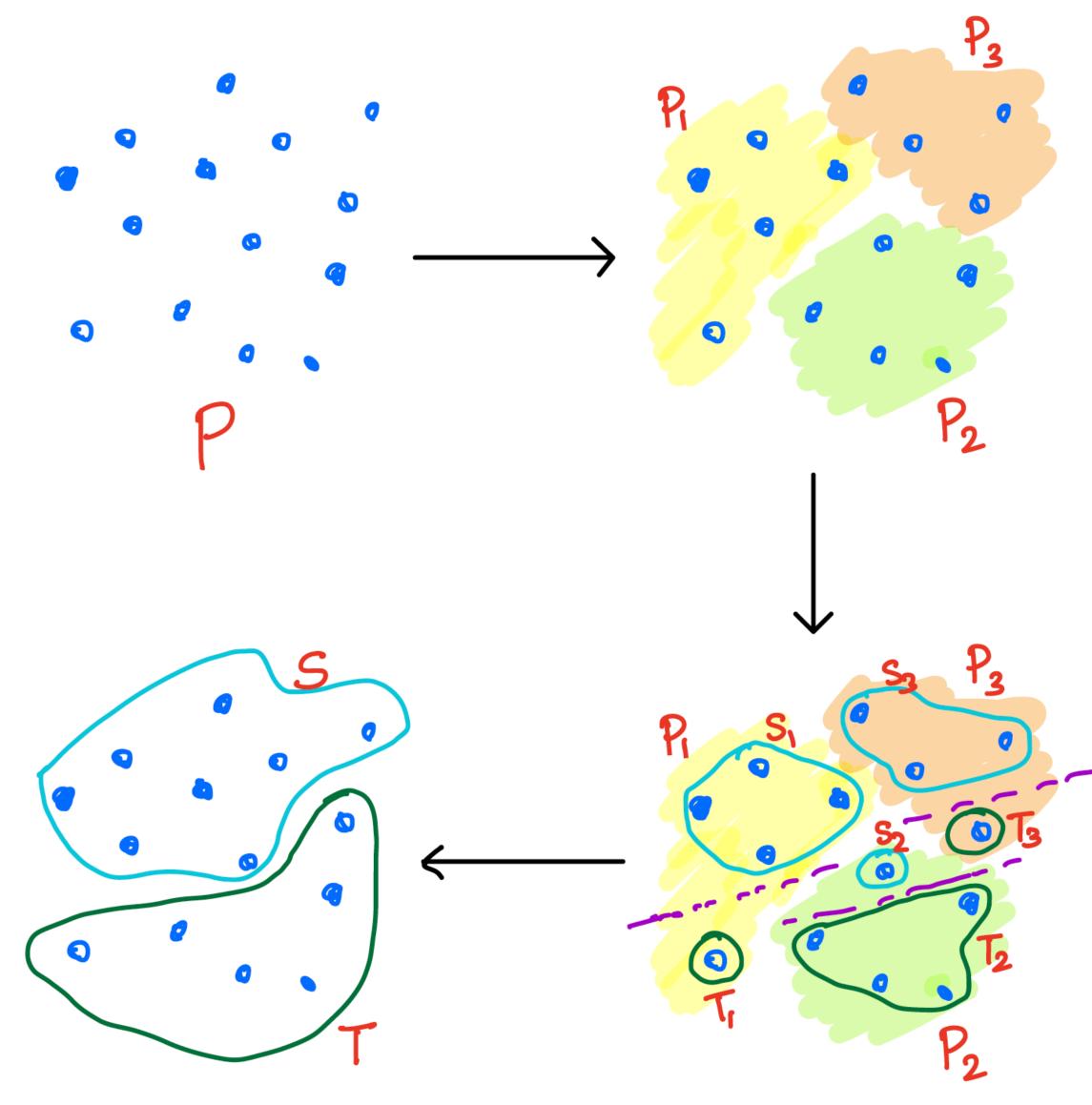
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2-means on *n* points can be solved in $2^{\omega n/3}$ time

- Enumerate all clustering (S_i, T_i) of P_i
- Construct graph H on $3 \cdot 2^{n/3}$ nodes
- Edge Weight of H is sum of pairwise intracluster distances
- Solve weighted triangle detection on $3 \cdot 2^{n/3}$ node graph H

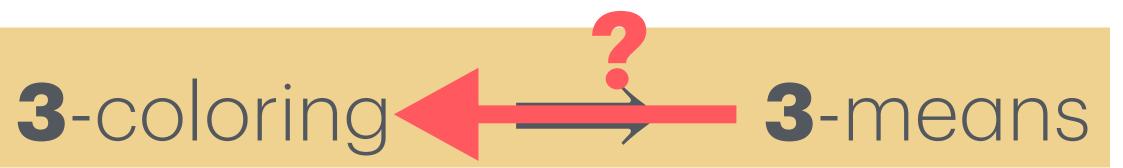


Open Directions





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Can we use ideas from 3-coloring algorithms to obtain $(2 - \varepsilon)^n$ time algorithm for 3-means?

Open Directions

Can we use ideas from 2-means algorithm to obtain $(2 - \varepsilon)^n$ time algorithm for 2-median or 2-center?

Thank you for engaging!